Modelling of Band Structure and Optical Properties of InAsP/InP Quantum Dots in Nanowires

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Chemical beam epitaxy (CBE) is known as efficient technological approach to grow quantum dots (QDs) in nanowires (NWs). In such a case the lateral size of the dot is limited by the width of the NW following the size of the seeding Au droplet, whereas the height of the nanostructure is controlled by the amount of deposited material. Compared to more common epitaxial self-assembled QDs embedded in a semiconductor matrix, CBE-grown QDs in NWs offer greater engineering capabilities for tailoring the energy levels and optical properties to meet requirements of specific application [1]. In addition, NWs geometry limits emission into the free-space modes in-plane and guide the emission in the vertical direction, which translates into increased light extraction efficiency resulting in brighter source with larger photon flux [2]. This is particularly important for nonclassical light sources, such as single photon emitters. However, a kind of drawback of this growth method is a deposition of a thin layer of QD material onto the bare substrate, i.e. in the areas beyond the NWs. This thin layer is expected to emit light which can overlap spectrally with emission from the QDs for certain thicknesses and compositions. Additionally, carriers could be trapped in it affecting overall carrier dynamics – both relaxation to the QDs and their emission. Therefore, it is crucial to better understand energy states of such a layer and its effect on QD emission.

The main objective of conducted research is to study theoretically the energy band structure of $InAs_xP_{1-x}$ QDs in InP NWs grown by CBE technique on InP substrate with different crystallographic orientations (1,0,0) and (1,1,1), which results in crystallization of the nanostructures in zinc blend or wurtzite structure, respectively. In particular, it is of interest if the thin $InAs_xP_{1-x}$ layer formed naturally during CBE growth of QDs, overlaps spectrally with QDs emission and what is the electronic structure of the system and its optical response. To calculate these properties versus various nanostructure geometries a commercial software Nextnano++ [3] is employed, i.e. an implementation of the 8-band $k \cdot p$ in three dimensions. Simulations are performed for realistic compositions and geometries following the structural data for several sets of samples: different QD heights and As content. As a result, the confined levels and probabilities of optical transitions are derived (without the excitonic effect) and compared with experimental results obtained from microphotoluminescence measurements.

[1] S. Battiato, S., et al, *Nanotechnology* **30**, 194004 (2019).
[2] J. Claudon, J. Bleuse, et al. *Nature Photon.* **4**, 174 (2010).
[3] https://nextnano.de/